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BASIC INSTABILITY MECHANISMS IN CHEMICALLY REACTING SUBSONIC AND SUPERSONIC FLOWS

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by

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This report summarizes the main results and conclusions of ~~obtained in a~~ research ~~program~~ on turbulent combustion. The main objective was to determine and elucidate the mechanisms governing turbulence-combustion interactions in different spectral regimes. Both theoretical and experimental investigations were conducted. Problems studied included: (1) Structure of disturbed flames; (2) Evolution of turbulence-combustion interactions; and (3) Thermal and flow structures of turbulent premixed V-flames at low Damköhler numbers. In an experimental investigation, Simultaneous measurements of velocity and temperature in premixed, rod-stabilized, lean methane-air V-flames demonstrated the presence of high-frequency fluctuations within slowly drifting flame brushes, leading to temporal changes in flame shapes, thicknesses and propagation speeds. Cross-correlation coefficients of these simultaneous signals assumed high values within the reaction zone, suggesting the possibility that these fluctuations might be induced by the same governing mechanism.

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effects of chemical reaction rate on the evolution of fluctuations in a reacting shear layer. The direct rate-augmentation effects due to reaction led to changes in phase relationships between the various fluctuations, resulting in turbulent energy and mass transport in a direction opposite to that suggested by the gradient model. Keywords: Reaction Kinetics; Energy transport; Thermal and flow structures; Methane/Ethane/Air.

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This report summarizes the main results and conclusions obtained in a research program on the study of turbulent combustion, conducted at the Massachusetts Institute of Technology with the support of the U.S. Air Force Office of Scientific Research under Grant AFOSR-83-0373. Detailed information may be found in the various publications listed in the Bibliography.

Despite recent important advance in the study of turbulent combustion, physical understanding of turbulence-combustion interactions was still obscure. The main objective of this research was to determine and elucidate the mechanisms governing these interactions in different spectral regimes. Both theoretical and experimental investigations were conducted. Problems studied during this grant period included: (1) Structure of disturbed flames (2) Evolution of turbulence-combustion interactions and (3) Thermal and flow structures of turbulent premixed V-flames at low Damköhler numbers. The results obtained are briefly described below.

(1) Structure of Disturbed Flames

In order to elucidate the mechanisms governing turbulence-combustion interactions, temporal development of spectral changes in the thermal structure of premixed, rod-stabilized, lean methane-air V-flames was examined as a quasi-laminar flame (in the absence of grid-generated turbulence) propagated into the wake region of a neighboring cylindrical rod of four different diameters (1.6, 0.89, 0.64 and 0.41 mm). Spectral density distributions of apparent all-pass mean-square temperature fluctuations within disturbed flames were compared with those within undisturbed

and turbulent flames (in the presence of turbulence-generating grids, the mesh size of which was equal to the corresponding disturbance rod diameter) at different distances downstream from the cylindrical flameholder. At 3 mm downstream, for example, before the wake of the disturbance rod interacted with the flame, the spectral structure within the disturbed flame resembled that within the undisturbed flame, while farther downstream due to interactions between the flame and the wake, the structure of the disturbed flame approached that of the corresponding turbulent flame, thus showing the temporal development of the disturbance effect from the neighboring cylinder.

The spectral density distributions in the presence of disturbance rods of different diameters were also compared. At 3 mm downstream, before wake-flame interactions, all the disturbed flames showed nearly the same structure in the high-frequency region. Farther downstream, however, the disturbed flame in the presence of the largest disturbance rod showed the highest spectral densities in the high-frequency region. These observations seemed to imply that the effects of the disturbance rods on the spectral structure were due to interactions of rate processes which became more pronounced with increasing disturbance-rod diameter and with increasing time as the flow moved downstream.

Comparison of simultaneous signals from two thermocouples spatially separated at a small distance apart indicated the presence of low-frequency flame movement, accompanied by higher-frequency fluctuations. The low-frequency fluctuations led to slow drifting of the flame across the temperature-monitoring station. Thus, the long-time signals obtained at a given spatial position in the laboratory-reference coordinates did

not originate from a fixed position within the flame brush. In order to shed light on the nature of the higher-frequency components at different "instantaneous" mean temperatures within the flame brush, the signals were analyzed within time intervals much shorter than the characteristic time of the low-frequency drifting but longer than that of the high-frequency components. One could then relate these fluctuations to the chemical effect at a mean temperature pertaining to this time interval and infer therefrom whether they were due to interactions between turbulence and combustion.

The RMS values of the high-frequency components were found to be closely related to the local "instantaneous" mean temperatures, being the highest within the reaction zone and lower near the unburned and the burned regions. Significant increases in the intensities of the high-frequency temperature fluctuations were observed in the presence of turbulence generated by grids and disturbance rods. Coupled with the effects of the equivalence ratios and of ethane addition to methane-air mixtures, one was led to believe that the high-frequency structure was affected by turbulence-combustion interactions.

Temporal development of the RMS temperature fluctuations within the high-frequency region was examined for undisturbed, disturbed, and turbulent flames. Consistent with the spectral density distributions discussed earlier, the RMS values for the disturbed flames were nearly the same as those for the undisturbed flames at small distances from the flameholder before the flames interacted with the wake of the disturbance rod. Farther downstream, on the other hand, the RMS values for the disturbed

flames approached those of the turbulent flames under the influence of the corresponding grid-generated turbulence. In other words, the high-frequency fluctuations were augmented to higher values in the presence of a larger disturbance rod, thus implying that the relevant interactions leading to the augmentation might also depend on the intensities and the scales of turbulence generated by the disturbance rods.

(2) Evolution of Turbulence-Combustion Interactions

Examination of the thermal and flow structure of premixed, rod-stabilized, lean methane/ethane/air V-flames showed the importance of turbulence-combustion interactions. In order to understand the mechanisms governing turbulence-combustion interactions, both theoretical and experimental investigations were conducted to study the evolution of these interactions.

(A) Theory

In the theoretical study, the stability of a chemically reacting shear layer with streamwise-velocity, concentration, and temperature gradients in the transverse direction under the influence of a longitudinal (or streamwise) pressure disturbance was examined. The pressure disturbance was assumed to be a travelling wave next to the unreacted region. In this two-dimensional model, it was expected that the interactions between the pressure and the density or entropy fluctuations would lead to the generation of vorticity, which was one of the three basic modes of fluctuations in turbulence.

The governing equations showed the following:

(a) The propagation of the pressure disturbance was affected by the presence of the mean transverse streamwise-velocity and temperature gradients as well as the fluctuations in the chemical reaction rate.

(b) The streamwise-velocity fluctuations were affected mainly by the mean transverse velocity gradient while the temperature, concentration, and vorticity fluctuations were affected mainly by the corresponding mean transverse gradient and the fluctuations in the chemical reaction rate. The effects of pressure fluctuations were comparatively small at low Mach numbers and for relatively long wavelength of the pressure disturbance with respect to the shear-layer thickness.

(c) The transverse velocity fluctuations were induced by the non-uniform distribution of the pressure fluctuations in the transverse direction.

(d) Fluctuations in the streamwise-velocity, concentration, temperature, and vorticity were induced through a "wrinkling-like" effect due to the coupling between the transverse velocity fluctuations and the corresponding mean transverse gradients.

(e) In addition to the "wrinkling-like" effect, there was the direct rate-augmentation effect on the concentration, temperature, and vorticity fluctuations due to chemical reaction.

(f) The direct chemical effects were found to depend on the activation energy, order, and enthalpy of reaction as well as the Damköhler first and third parameters.

Numerical solutions of the governing equations for the case of small shear-layer thickness relative to the wavelength of the pressure disturbance showed that the flow was always unstable, leading to amplification of all fluctuations. The case of a nonreacting shear layer with no transverse temperature gradient was found to be the most unstable. In the presence of the transverse temperature gradient, with or without chemical reaction, the flow became less unstable. Nevertheless, the flow was more unstable with chemical reaction, with increasing amplification rate for higher activation energy and faster chemical reaction rate. Also, with increasing wave number or decreasing wavelength of the pressure disturbance, the amplification rate per second increased while the amplification rate per cycle decreased.

In order to elucidate the coupling mechanism governing turbulence-combustion interactions, the phase relationships between the various fluctuations were examined. Comparisons of the complex eigenfunctions representing the various fluctuations in the phase plane at different positions within the shear layer with and without chemical reaction showed that the main effect of chemical reaction was to cause large changes in the phase angles, thus leading to rather complex coupling between the various fluctuations.

Cross-correlations of the transverse-velocity fluctuations and temperature or concentration fluctuations with and without chemical reaction were also examined. For non-reacting flows, the correlations remained negative within the entire shear layer, indicating that the turbulent energy or mass transport could be related to the mean transverse temperature or concentration gradient on the basis of an "eddy-diffusivity"

model. On the other hand, with chemical reaction, the correlations were positive in that part of the shear layer closer to the unreacted region, indicating the inappropriateness of the gradient model to account for the turbulent transport.

In the case of cross-correlations of the streamwise- and the transverse-velocity fluctuations, however, they remained negative within the entire shear layer with or without chemical reaction, indicating positive Reynolds stresses.

(B) Experiments

In order to shed light on the nature of the turbulence-combustion interactions, experiments were conducted to examine the relationships between simultaneous instantaneous temperatures and velocities (either normal or tangential to the flame brush) within the turbulent flame. This study showed that the high-frequency fluctuations in temperatures and normal velocities were highly correlated and were associated with changes in flame shapes, thicknesses, and propagation speeds. Furthermore, their RMS values were higher within the reaction zone than in either the cold or hot regions. However, the fluctuations in tangential velocities were less well correlated with temperatures and their RMS values remained almost constant within the flame brush.

The evolution of turbulence-combustion interactions was examined in three types of simultaneous measurements:

(a) dual-thermocouple measurements at different distances apart

(b) normal velocity-temperature measurements

(c) dual-thermocouple in conjunction with normal or tangential velocity measurements.

They are described below.

(a) Simultaneous Dual-Thermocouple Measurements

Instantaneous temperatures within turbulent, premixed, lean, chemically pure methane/air, unconfined V-flames stabilized behind a 2.1 mm-diameter cylindrical flameholder were monitored simultaneously by the use of two fine-wire, frequency-compensated thermocouples at different distances apart. "Instantaneous" mean temperature profile of the slowly drifting flame was determined by analyzing the variation of the corresponding mean temperatures at the two positions. The instantaneous temperature profiles, however, assumed different shapes and thicknesses in the presence of the higher-frequency fluctuations. The instantaneous temperatures rose in the region where the average temperature gradient between the two positions was higher than the value corresponding to the "instantaneous" mean temperature profile (or where the flame was relatively thinner) and dropped in the region where the average gradient was lower, thus leading to the observed higher-frequency temperature fluctuations. Furthermore, the rates of the temperature rise and drop assumed maximum values at the instants when the temperature gradient was the largest (or the turbulent flame was the thinnest) and the smallest (or the flame was the thickest), respectively. Since the temperature gradient and the flame thickness were in some respects related to the turbulence intensity, the temperature rise and drop which resulted in the high-frequency fluctuations were presumably due to varying degrees

of turbulence-combustion interactions.

Examination of the spatial cross-correlations of the simultaneous temperatures at different distances apart showed that the integral scale of the eddies responsible for the high-frequency fluctuations was less than 1 mm and that for the low-frequency drifting was larger. (For comparison, note that the corresponding laminar-flame thickness at an equivalence ratio of 0.75 reported in the literature was about 1.5 mm.) These results seemed to be consistent with the conceptual model proposed by Damköhler* that rate-augmentation within turbulent flames was due to eddies smaller in size than the laminar-flame thickness.

(b) Simultaneous Normal Velocity-Temperature Measurements

Similar to the temperature measurements noted in earlier experiments, simultaneous measurements of velocity (by a Laser-Doppler-Velocimetry system) in a direction normal to the flame brush also showed the presence of high-frequency fluctuations within slowly drifting flame brushes, thus suggesting a structure different from that of a simple wrinkled discontinuity. Both the velocity and the temperature fluctuations gave maximum RMS values at a position somewhere between the unreacted and the product gases. Cross-correlation coefficients of the simultaneous temperature and normal-velocity fluctuations remained positive within the entire flame brush, thus indicating the inappropriateness of the gradient

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*Damköhler, G. (1940). Der Einfluss der Turbulenz auf die Flammengeschwindigkeit in Gasgemischen. Z. Elektrochem. Angew. Phys. Chem. 46, 601; (1947). Engl. trans.: The effect of turbulence on the flame velocity in gas mixtures. NACA Tech. Mem. 1112.

model to account for the turbulent energy transport (in agreement with the prediction near the unreacted region from the theoretical study discussed earlier). Both the apparent and the "instantaneous" V'-T' cross-correlation coefficients assumed rather high values (0.8-0.9, maximum) within the reaction zone, suggesting the possibility that these fluctuations might be induced by the same governing mechanism (which, according to the theory, was due to the coupling between chemical kinetics and turbulence).

The "instantaneous" mean velocities and temperatures within the flame brush were found to fluctuate at low frequencies as the result of the flame drifting across the signal-monitoring station. Should the flame be simply a wrinkled discontinuity, they would assume only values corresponding to the unreacted and the product gases. However, a turbulent structure was found to be present, with the "instantaneous" velocities varying almost linearly with the "instantaneous" temperatures. Since the velocities were measured in a direction normal to the flame brush, this linear relationship was expected because the mass flux crossing the flame brush should remain the same.*

Spectral density distributions of mean-square temperature and simultaneous mean-square velocity fluctuations were examined for flames with and without grid-generated turbulence. In all cases, remarkable similarity was observed over the entire spectral regime between the velocity and the temperature fluctuations. Together with the earlier

*Note that the density-temperature product was assumed to remain constant for almost the same pressure across the flame brush.

observation on the rather high values of the normalized cross-correlation coefficients, this spectral similarity gave further support to the postulation that both the velocity and the temperature fluctuations were induced by the same governing mechanisms.

Comparisons of the spectral density distributions of apparent all-pass mean-square velocity fluctuations just upstream of the flame brush and at a position of maximum RMS values showed a significant increase within the flame brush, suggesting the presence of flame-generated turbulence.

Probability density functions across the flame brush for the simultaneous temperature and velocity fluctuations were also examined. Near the unburned and the burned regions, the temperatures and the velocities corresponded essentially to those of the ambient and the products, respectively. Within the flame brush, however, significant contributions from intermediate states were observed. Even at the location of the maximum RMS values, their shapes were not bimodal, confirming the earlier observation that the turbulent flame structure was not one of the simple wrinkled discontinuity.

The variation of the corresponding instantaneous velocities and temperatures showed that at a given temperature the velocity was higher in a region where the temperature was rising. According to the previous discussion on dual-thermocouple measurements, the velocity was higher in a region where the average temperature gradient was larger than that corresponding to the "instantaneous" mean temperature profile or where the flame was thinner.

The instantaneous mass flux was related to the ratio of the

corresponding velocity and temperature, if one assumed that the density-temperature product remained constant for almost the same pressure across the flame brush. The variation of the simultaneous instantaneous values showed that at a given temperature the mass flux was higher in a region where the temperature was rising or where the average temperature gradient was larger than that corresponding to the "instantaneous" mean temperature profile. Noting that the mass flux was related to the turbulent flame-propagation speed, one concluded that the propagation speed was higher in a region where the flame was relatively thinner. Thus, due to turbulence-combustion interactions, the turbulent flame changed its structure and propagation speed.

(c) Simultaneous Dual-Thermocouple/Normal or Tangential Velocity Measurements

In order to further elucidate the evolution of the turbulence-combustion interactions, their effects on the flame structure and propagation speeds, and their governing mechanisms, experiments were performed to examine the relationships between the instantaneous velocities, in directions normal (V) and tangential (U) to the flame brush, and temperatures at two other neighboring locations. One thermocouple T_1 was placed 1 mm vertically above the LDV station and another thermocouple T_2 0.4 mm apart from T_1 in the horizontal direction away from the hot products. The projections of the trajectories $V/T_1/T_2$ onto the respective planes T_2, T_1; V, T_2; and V, T_1 were examined. Similar to the results described earlier, the projection on the (T_2, T_1) plane described a counter-clockwise trajectory, with both T_1 and T_2 rising in a region of larger temperature difference

or average gradient and dropping in a region of smaller temperature gradient. Also, the projection on the (V, T_2) plane described a clockwise trajectory, with higher velocity in a region where the temperature was rising or where the average temperature gradient was larger and the flame was thinner. On the other hand, the projection on the $(V-T_1)$ plane did not seem to exhibit any definitive pattern.

Despite increasing apparent mean normal velocities across the flame brush with rising temperatures, the apparent mean tangential velocities remained almost constant. The apparent RMS temperature and normal-velocity fluctuations assumed distinct maximum values somewhere within the reaction zone, while the RMS tangential-velocity fluctuations increased only slightly with rising temperatures within the flame.

Similar behaviors were observed for the "instantaneous" mean values and the high-frequency RMS fluctuations.

Normalized cross-correlation coefficients of the simultaneous velocity and temperature fluctuations within the high-frequency region at different instantaneous mean temperatures were also examined. They remained positive within the flame for both the normal- and the tangential-velocity fluctuations, thus indicating the inappropriateness of the gradient model to account for the turbulent energy transport. Furthermore, the coefficients involving normal velocity components assumed higher values than those involving tangential components.

Spectral density distributions of apparent all-pass mean-square normal- and tangential-velocity fluctuations were compared at three different positions within the flame. For the normal velocity component,

the values at the position of the maximum RMS fluctuations were significantly higher than those in the hot products and the cold reactants, thus suggesting the presence of flame-generated turbulence. On the other hand, the distribution for the tangential velocity component remained almost the same across the flame, implying that the nature of the turbulence-combustion interactions in the tangential direction may be different from that in the normal direction.

(3) Thermal and Flow Structures of Turbulent Premixed V-Flames at Low Damköhler Numbers

Simultaneous measurements of temperatures and velocities within a premixed, lean methane/air turbulent V-flame at low Damköhler numbers showed that its structure was one of a slightly wrinkled "thick" flame. The wrinkle wavelength was about 32 mm, the amplitude of the order of 0.5 mm, and the flame thickness on the average 1.5 mm (which was comparable to the laminar-flame thickness). The larger apparent flame brush thickness at the measurement station of approximately 4.2 mm was the result of low-frequency flame drifting. The accompanying high-frequency fluctuations within the slowly drifting flame brush led to changes in the most probable instantaneous flame shapes, with steeper spatial temperature gradients and thinner flames when the temperatures were rising than when they were falling. Furthermore, the high-frequency RMS temperature and normal-velocity fluctuations assumed maximum values near the inflection points of the respective temperature and velocity profiles.

On the basis of the temporal changes in the average temperatures and temperature gradients between two positions separated at 0.3 mm apart normal to the flame brush, the speed of the flame movement in the laboratory-coordinate system could be estimated. Comparison of the computed flame speed with the measured temperatures showed the presence of similar high-frequency fluctuations. Furthermore, their cross-correlation coefficients at different delay times could be represented by an odd function with peak values at about -0.8 and 1.0 ms. The crossing of the correlation curve at zero delay time also suggested that the flame-speed fluctuation led the temperature fluctuation by about 90 degrees.

The effect of flame on flow turbulence was non-isotropic and not the same in different spectral regimes. Within the flame, the turbulence component normal to the flame brush increased mainly through thermal expansion and turbulence-combustion interactions, while the tangential component increased in intensity presumably through energy transport from the normal component. Turbulence energy augmentation across frequency spectrum was not constant and varied with the upstream turbulence.

Flame chemistry was altered through changes in equivalence ratio and varying methane/ethane compositions. Although fluctuation intensities were higher for richer (lean) flames, the distributions of the spectral densities did not change across the spectra with the equivalence ratio. The effect of ethane addition to methane/air mixtures showed a non-monotonic relationship between mixture composition and thermal fluctuation intensity, with the highest intensity occurring at 10%-ethane addition. However, the normalized spectral density distributions were about the same for different methane/ethane/air compositions.

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3. Toong, T.Y. and Chang, C.T., "Thermal Structure of Turbulent Premixed Rod-Stabilized V-Flames", the Fall Technical Meeting, Eastern Section, Combustion Institute, December 1986.
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5. Toong, T.Y. and Chang, C.T., "Thermal Structure of Turbulent Premixed Rod-Stabilized V-Flames at Low Damköhler Numbers", in preparation.
6. Chang, C.T., "Flow and Thermal Structures of a Turbulent V-Flame at Low Damköhler Numbers", Ph.D. Thesis, Department of Mechanical Engineering, M.I.T., June 1988.
7. Chang, C.T. and Toong, T.Y., "Thermal and Flow Structures of a Turbulent Premixed Methane/Air V-Flame at Low Damköhler Numbers", in preparation.

APPENDIX

(1) Professional Personnel

Professor T.Y. Toong, Principal Investigator

Dr. G.E. Abouseif, Co-Investigator

Mr. C.T. Chang, Research Assistant

Mr. Z.Y. Du, Research Fellow

Mr. R.L. Godown, Senior

(2) Advanced Degrees Awarded

(i) Z.Y. Du S.M. Department of Mechanical Engineering, M.I.T., May 1985.

"Instability Analysis in a Reacting Shear Layer"

(ii) C.T. Chang Ph.D. Department of Mechanical Engineering, M.I.T., September 1988.

"Flow and Thermal Structures of a Turbulent V-Flame at Low Damköhler Numbers"

(3) Spoken Papers and Other Presentations

(i) A seminar on Turbulence-Combustion Interactions was presented by T.Y. Toong at the Massachusetts Institute of Technology on April 26, 1984.

(ii) A presentation on Turbulence-Combustion Interactions — Theory and Experiments was made by T.Y. Toong at the 1985 AFOSR/ONR Contractors Meeting on Combustion at the California Institute of Technology on July 25, 1985.

(iii) A presentation on Thermal Structure of Turbulent Premixed Rod-Stabilized V-Flame was made by T.Y. Toong at the 1986 Fall Technical Meeting, Eastern Section of the Combustion Institute on December 15, 1986.

(iv) A seminar on Evolution of Turbulence-Combustion Interactions — Theory and Experiments was made by T.Y. Toong at the Yale University on April 2, 1987.

(v) A presentation on Evolution of Turbulence-Combustion Interactions was made by T.Y. Toong at the 1987 AFOSR/ONR Contractors Meeting on Propulsion Research at the Pennsylvania State University on June 22, 1987.